

# Extended universality of the surface curvature in equilibrium crystal shapes

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## Abstract

We investigate the universal property of curvatures in surface models which display a flat phase and a rough phase whose criticality is described by the Gaussian model. Earlier we derived a relation between the Hessian of the free energy and the Gaussian coupling constant in the six-vertex model. Here we show its validity in a general setting using renormalization group arguments. The general validity of the relation is confirmed numerically in the RSOS model by comparing the Hessian of the free energy and the Gaussian coupling constant in a transfer matrix finite-size-scaling study. The Hessian relation gives clear understanding of the universal curvature jump at roughening transitions and facet edges and also provides an efficient way of locating the phase boundaries.

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## I. INTRODUCTION

The theory of equilibrium crystal shapes (ECS) is well established [1–4]. Consider a macroscopic amount of solid in coexistence with and surrounded by its own fluid phase. The shape of the solid region is obtained by minimizing the total free energy of the solid-fluid interface subject to the fixed-volume constraint. This leads to the Wulff construction for ECS. Especially if one focuses on a particular direction, say the  $z$  direction, the crystal surface is defined by the height  $z(\mathbf{r})$  of the surface with respect to the position  $\mathbf{r} = (x, y)$  in a reference plane. If the surface with slope  $\mathbf{m}$  costs a free energy  $\sigma(\mathbf{m})$  per unit base area, the ECS is given by [2]

$$\lambda z(\mathbf{r}) = f(-\lambda \mathbf{r}) , \quad (1)$$

where  $2\lambda$  is the pressure difference between the two phases [1] and  $f(\mathbf{h})$  is the Legendre transform of  $\sigma(\mathbf{m})$ :

$$f(\mathbf{h}) = \min_{\{\mathbf{m}\}} \{ \sigma(\mathbf{m}) - \mathbf{h} \cdot \mathbf{m} \} . \quad (2)$$

Here,  $\mathbf{h}$  is the surface-tilting field conjugate to the surface slope. Equation (1) states that the surface free energy as a function of the surface-tilting field is itself the height of the surface from the base plane up to appropriate scaling of coordinates.

Using this connection, the thermal evolution of the equilibrium shape of a face-centered-cubic (fcc) crystal or a body-centered-cubic (bcc) crystal has been studied through the body-centered solid-on-solid (BCSOS) model which is equivalent to the six-vertex model [4–6]. The surface slope and the surface-tilting field in the BCSOS model correspond to the polarization and the electric field in the six-vertex model, respectively. The six-vertex model displays several ordered phases with ferroelectric or anti-ferroelectric order and a disordered phase [7,8]. The disordered phase is a critical phase. Its scaling behavior is described by the Gaussian model, and is parameterized by the Gaussian coupling constant  $g$  or the stiffness constant  $K$  [9]. At zero fields a Kosterlitz-Thouless (KT) type roughening transition takes place [8].

Below the roughening temperature  $T_R$ , the system is ordered with zero polarization when the field is small but it becomes rough with non-zero polarization beyond a critical value of the electric field. This transition is in the Pokrovsky–Talapov (PT) transition universality class [7,10]. The PT transition is characterized by the specific heat exponent  $\alpha = 1/2$  [10], which implies that the free energy scales as  $f \sim |\mathbf{h} - \mathbf{h}_c|^{3/2}$ .

Equation (1) enables one to identify the ordered and the disordered phases to facet and rounded regions in ECS, respectively. Below  $T_R$  a facet appears surrounded by rounded vicinal surface. The rounded region in the ECS is rough in the sense that the height-difference correlation function behaves as

$$\langle (z(\mathbf{r}) - z(\mathbf{r}'))^2 \rangle \sim \frac{1}{2\pi^2 g} \ln |\mathbf{r} - \mathbf{r}'| .$$

The PT transition line corresponds to the facet edge and the crystal profile near the facet edge is given by  $z \sim (x_\perp - x_{\perp 0})^{3/2}$ , where  $x_\perp$  is a coordinate perpendicular to the facet edge and  $x_{\perp 0}$  is the facet-edge position.

A measurable quantity of physical importance is the surface curvature  $\kappa \equiv \sqrt{z_{x,x}z_{y,y} - z_{x,y}^2}$ , where the subscripts denote partial derivatives. From Eq. (1), the surface curvature is related to the Hessian of the free energy as

$$\kappa = \lambda \sqrt{H[f(\mathbf{h} = -\lambda \mathbf{r})]} = \frac{\lambda}{\sqrt{H[\sigma(\mathbf{m})]}} . \quad (3)$$

The Hessian of a function  $F(\mathbf{x})$  is defined by

$$H[F(\mathbf{x})] = \det \begin{vmatrix} F_{x_1,x_1} & F_{x_1,x_2} \\ F_{x_2,x_1} & F_{x_2,x_2} \end{vmatrix} .$$

The second equality in Eq. (3) follows from the identity  $H[f(\mathbf{h})]H[\sigma(\mathbf{m})] = 1$ . It has been predicted [11] and measured experimentally [12] that the curvature displays a universal jump at the roughening transition with discontinuity

$$(\Delta\kappa)_{\text{KT}} = \frac{2}{\pi} \frac{\lambda d^2}{k_B T_R} , \quad (4)$$

where  $d$  is the distance between the crystal planes. It is also expected [13] that, for  $T < T_R$ , there is universal curvature jump at the facet edge with discontinuity

$$(\Delta\kappa)_{\text{PT}} = \frac{1}{\pi} \frac{\lambda d^2}{k_B T} . \quad (5)$$

These universal jumps are attributed to the universal nature of the roughening transition and the PT transition. Surface fluctuations without surface-tilting field are assumed to be described by the Gaussian model and the universal jump  $(\Delta\kappa)_{\text{KT}}$  is related to the jump of the stiffness constant at the KT transition [11]. On the other hand, fluctuations of the vicinal surface near the facet edge are described by the one-dimensional free fermion model where the world lines of fermions are interpreted as step excitations in the surface [13]. It explains the universal jump  $(\Delta\kappa)_{\text{PT}}$  at the facet edge.

In a recent paper [9] on the six-vertex model, an exact relation has been found between the Hessian of the six-vertex model free energy and the Gaussian coupling constant  $g$  in the rough phase. The relation is given as  $\bar{\text{H}}[f(\mathbf{h})] = (\frac{2}{\pi g})^2$ , where  $\bar{\text{H}}$  is the Hessian of the six-vertex model free energy in units of  $k_B T$  with respect to the dimensionless surface-tilting field. When one restores the dimensions, this relation becomes

$$\text{H}[f(\mathbf{h})] = \left( \frac{2d^2}{k_B T \pi g} \right)^2 . \quad (6)$$

The Gaussian coupling constant determines the scaling exponents of various correlations and controls the finite-size-scaling (FSS) behaviors, i.e., a set of excitation energies  $\Delta E$  of the transfer matrix, defined for a system with strip of width  $N$ , satisfies the FSS form

$$\text{Re}(\Delta E) = \frac{2\pi\zeta''}{N} \left( \frac{m^2}{2g} + \frac{gn^2}{2} + \mathcal{N} + \bar{\mathcal{N}} \right) , \quad (7)$$

where  $\zeta''$  is the imaginary part of the anisotropy factor,  $(\mathcal{N}, \bar{\mathcal{N}})$  a non-negative set of integers, and  $(m, n)$  the level index, which takes integer values (see [9,14] for details). If one combines Eqs. (3) and (6), one gets

$$\kappa = \frac{2\lambda d^2}{\pi k_B T} \frac{1}{g} . \quad (8)$$

It was found that  $g = 1$  at the KT-type roughening transition in the fcc (110) surface and  $g = 2$  at the PT-type facet edges [9]. If one uses them in Eq. (8), the universal jumps in Eqs. (4) and (5) are obtained. Relation (6) or equivalently (8) is quite general in the sense that it does apply to the entire rough phase as well as at the phase transition points of the six-vertex model. A natural question that arises is whether such general relation is universal, in other words, whether it holds in other model systems too. This paper addresses to this question, and the results are affirmative.

In Sec. II we introduce general models for crystal surfaces which display phase transitions between flat and rough phases, and present renormalization group (RG) arguments that the Hessian of the free energy is the scale-invariant quantity. It yields the relation between the Hessian of the free energy and the Gaussian coupling constant in the rough phase. The result is given in Eq. (27). Combining it with the theory of the ECS, we obtain the relation between the surface curvature and the Gaussian coupling constant. To check the general theory, we present numerical results for the restricted solid-on-solid (RSOS) model in Sec. III. The Gaussian coupling constants, obtained in the FSS study from the transfer matrix spectra, is compared with the value obtained from the Hessian of the free energy. This confirms the validity of the universal relation. In Sec. IV, we discuss implications of the results and give brief summary.

## II. RENORMALIZATION GROUP THEORY

Consider a solid-on-solid (SOS) type model for a two-dimensional crystal surface, where the surface is defined by height  $z_i$  at each site  $i$  on a substrate of size  $L_1 \times L_2$  parallel to one of its crystal planes. The sites consist of projections of all lattice points on to the substrate and form a two-dimensional lattice. Figure 1 shows three examples of such substrates for sc (001), bcc (001), and sc (111) surfaces, respectively. In SOS type model the height is a single-valued function; there are no overhangs. The height at a given site can change by an integer multiple of the lattice constant  $a_3$  in the  $z$  direction. Due to the crystal structure

there may be  $p$  distinct classes of crystal planes parallel to the substrate, with inter-plane spacing  $d = a_3/p$ . In that case substrate sites are separated into  $p$  sublattices and  $z_i$  takes the values  $(l_i d + \text{integer} \times a_3)$  if the site  $i$  belongs to the  $l_i$ th sublattice ( $l_i = 1, 2, \dots, p$ ). For examples shown in Fig. 1,  $p = 1$ ,  $p = 2$ , and  $p = 3$  in Fig. 1 (a), (b), and (c), respectively. Fcc (110) surfaces also have  $p = 2$ .

At low temperatures the surface will be in a flat phase. Steps which separate domains of flat regions are the basic excitations and thermodynamic properties of the surface are described by a general Hamiltonian  $\mathcal{H}$  which consists of the step-creation energy ( $\mathcal{H}_S$ ), the interaction energy between steps ( $\mathcal{H}_I$ ), and the surface-tilting energy ( $\mathcal{H}_T$ ) which controls the average slope of the surface. They are given by

$$\mathcal{H}_S = J \sum_{\langle i,j \rangle} |z_i - z_j|^2 \quad (9)$$

$$\mathcal{H}_T = -h_1(\Delta z)_1 L_2 - h_2(\Delta z)_2 L_1, \quad (10)$$

where  $\langle i, j \rangle$  denotes the pair of nearest neighbor sites,  $J$  is the step energy,  $(\Delta z)_1$  ( $(\Delta z)_2$ ) is the total difference in height across the lattice in the 1 (2) direction, i.e., the difference in height between two sites  $i = (L_1, y)$  and  $i = (0, y)$  ( $i = (x, L_2)$  and  $i = (x, 0)$ ) of the substrate, and  $\mathbf{h} = (h_1, h_2)$  is the surface-tilting field. The explicit form of  $\mathcal{H}_I$  is not important in the following analysis. Since long-wavelength fluctuations are dominant in the rough surface, we neglect height fluctuations inside the unit cell of the two-dimensional lattice and introduce a coarse-grained height  $\bar{z}_j$  which is the average height inside the unit cell containing sites  $i$  around the site  $j$ . (The coarse-graining scheme for the sc (111) surface is given in Ref. [15].) Then  $\{\bar{z}_j\}$  takes integer multiples of  $d$ .

The free energy as a function of the surface slope  $\mathbf{m} = (m_1, m_2)$  per unit base area is given by

$$\sigma(\mathbf{m}) = -\frac{k_B T}{(L_1 L_2)} \ln \mathcal{Z} \quad (11)$$

with the partition function  $\mathcal{Z} = \sum'_{\{\bar{z}_i\}} e^{-\beta(\mathcal{H}_S + \mathcal{H}_I)}$ , where the prime denotes the sum over all surface configurations satisfying the shifted boundary condition (SBC)  $(\Delta \bar{z})_i = m_i L_i$

( $i = 1, 2$ ).  $\mathbf{m}$  and  $\mathbf{h}$  are related as  $\mathbf{h} = \nabla_{\mathbf{m}}\sigma(\mathbf{m})$ . Using the Poisson sum formula

$$\sum_{n \in \delta \mathbf{Z}} F(n) = \sum_{n \in \mathbf{Z}} \int_{-\infty}^{\infty} \frac{d\phi}{\delta} F(\phi) e^{2\pi i n \phi / \delta},$$

one can replace the discrete sum over  $\bar{z}$  by integral over continuous field  $\phi$  with additional harmonic terms. The partition function in the continuum limit is then put in the form

$$\mathcal{Z} = \int_{SBC} [\mathcal{D}\phi] e^{-\beta \mathcal{H}_{\text{eff}}[\phi(\mathbf{r})]}, \quad (12)$$

where the effective Hamiltonian is given by

$$\beta \mathcal{H}_{\text{eff}} = \frac{K}{2} \int d^2 \mathbf{r} |\nabla \phi|^2 + \beta \mathcal{H}' \quad (13)$$

with

$$\beta \mathcal{H}' = - \sum_n V_n \int d^2 \mathbf{r} \cos \left( \frac{2\pi n \phi(\mathbf{r})}{d} \right) + \beta \mathcal{H}_{\text{I}}[\phi(\mathbf{r})]. \quad (14)$$

The functional integral in Eq. (12) is taken over the field satisfying the SBC

$$\phi(\mathbf{r} + L_i \mathbf{e}_i) = \phi(\mathbf{r}) + m_i L_i, \quad (15)$$

where  $\mathbf{e}_1$  ( $\mathbf{e}_2$ ) is the unit vector in the 1 (2) direction. Here we assume for simplicity that the substrate is a square lattice whose lattice constants in 1 and 2 directions are the same so that the stiffness constant  $K = 2\beta J$  is a scalar. We will discuss later the more general case where the stiffness constant is a tensor. The sine-Gordon (SG) terms  $V_n \cos(2\pi n \phi / d)$  account for the discreteness of heights.

The effective Hamiltonian  $\mathcal{H}_{\text{eff}}$  is the starting point of our RG arguments for the universal relation between the Hessian of the free energy and the Gaussian coupling constant. The RG theory for  $\mathcal{H}_{\text{eff}}$  with  $\mathbf{m} = 0$  and in the absence of  $\mathcal{H}_{\text{I}}$  is well established [16–18]. At high temperatures where the surface is rough, all SG terms are irrelevant and hence  $V_n$ 's renormalize to zero and  $K$  renormalizes to a fixed-point value  $K^*$ . And at low temperatures the leading harmonics becomes relevant and the surface is flat. At the roughening transition  $K^*$  takes the universal value of  $\frac{\pi}{2}$ . The RG transformation for  $\mathcal{H}_{\text{eff}}$  in the presence of

$\mathcal{H}_1$  and nonzero  $\mathbf{m}$  can be performed similarly in the following way: (i) First introduce a field variable  $\phi_0(\mathbf{r}) \equiv \phi(\mathbf{r}) - \mathbf{m} \cdot \mathbf{r}$ , which satisfies the periodic boundary condition (PBC)  $\phi_0(\mathbf{r} + L_i \mathbf{e}_i) = \phi_0(\mathbf{r})$ . The partition function is then re-written as a functional integral over the field  $\phi_0$  as

$$Z = e^{-\frac{1}{2}K|\mathbf{m}|^2 L_1 L_2} \int_{PBC} [\mathcal{D}\phi_0] \exp \left\{ -\frac{K}{2} \int d^2 \mathbf{r} |\nabla \phi_0|^2 - \beta \mathcal{H}'[\phi_0(\mathbf{r}) + \mathbf{m} \cdot \mathbf{r}] \right\} .$$

(ii) The field  $\phi_0$  is expanded in a Fourier integral as

$$\phi_0(\mathbf{r}) = \int_{|\mathbf{p}| < \Lambda} \frac{d^2 \mathbf{p}}{(2\pi)^2} \tilde{\phi}_0(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{r}} ,$$

where  $\Lambda$  is the ultraviolet cutoff, and is separated into two parts  $\phi'_0(\mathbf{r})$  and  $\phi''_0(\mathbf{r})$  such that  $\phi_0(\mathbf{r}) = \phi'_0(\mathbf{r}) + \phi''_0(\mathbf{r})$  and  $\phi'_0$  ( $\phi''_0$ ) has only  $0 < |\mathbf{p}| < \Lambda'$  ( $\Lambda' < |\mathbf{p}| < \Lambda$ ) components of the Fourier modes. Then the partition function is decomposed as

$$Z = e^{-\frac{1}{2}K|\mathbf{m}|^2 L_1 L_2} \int_{PBC} [\mathcal{D}\phi'_0] e^{-\frac{K}{2} \int d^2 \mathbf{r} |\nabla \phi'_0|^2} \times \int_{PBC} [\mathcal{D}\phi''_0] \exp \left\{ -\frac{K}{2} \int d^2 \mathbf{r} |\nabla \phi''_0|^2 - \beta \mathcal{H}'[\phi'_0(\mathbf{r}) + \mathbf{m} \cdot \mathbf{r} + \phi''_0(\mathbf{r})] \right\} .$$

(iii) A partial integration over the fluctuations of  $\phi''_0$  is performed and the remaining field  $\phi'_0$  is transformed back to  $\phi'(\mathbf{r}) \equiv \phi'_0(\mathbf{r}) + \mathbf{m} \cdot \mathbf{r}$ , which corresponds to the long-wave-length fluctuation part of  $\phi(\mathbf{r})$ . (iv) The RG transformation is completed by rescaling the momenta or the coordinate and the field as

$$\begin{aligned} \mathbf{p} &\rightarrow b \mathbf{p} \quad \text{or} \quad \mathbf{r} \rightarrow \mathbf{r}/b , \\ \phi'(\mathbf{r}) &\rightarrow \zeta \phi_{new}(\mathbf{r}/b) \end{aligned} \tag{16}$$

with the scale factor  $b = \Lambda/\Lambda'$ . The scale factor  $\zeta$  for the field will be taken to be 1 to describe the Gaussian fixed point for the rough phase. Combining Eqs. (15) and (16), one can see that  $\phi_{new}$  satisfies the SBC

$$\phi_{new}(\mathbf{r} + \frac{L_i}{b} \mathbf{e}_i) = \phi_{new}(\mathbf{r}) + b m_i \left( \frac{L_i}{b} \right) , \tag{17}$$

which implies that the slope is renormalized to



$$\mathbf{m}' = b\mathbf{m} . \quad (18)$$

Under the RG transformation the free energy is transformed as

$$\sigma(\mathcal{P}, \mathbf{m}) = b^{-2}\sigma(\mathcal{P}', \mathbf{m}') + G , \quad (19)$$

where  $\mathcal{P}$  denotes a set of model parameters,  $G$  is the analytic background depending on  $\mathcal{P}$  and possibly on  $\mathbf{m}$ , and  $\mathcal{P}'$  is the set of the renormalized model parameters. Let us focus on step (iii) where the partial integration over  $\phi_0''$  is performed, which results in the renormalization of model parameters. However, the difference between the  $\mathbf{m} = 0$  case is that the argument of  $\mathcal{H}'$  is replaced by  $\phi_0' \rightarrow (\phi_0' + \mathbf{m} \cdot \mathbf{r})$ , which does not participate in the integral. Therefore  $K$  and the functional form of  $\mathcal{H}'$  renormalize in the same way as at  $\mathbf{m} = 0$ , and the renormalized values of  $\mathcal{P}'$  and  $G$  are only a function of  $\mathcal{P}$  independent of  $\mathbf{m}$ . As a consequence, one can readily see that the Hessian of the free energy is the scale-invariant quantity:

$$\text{H}[\sigma(\mathbf{m})] = \text{H}[\sigma(\mathbf{m}')] . \quad (20)$$

After successive applications of the RG transformation infinitely many times, the Hamiltonian is renormalized to

$$\beta\mathcal{H}^* = \frac{1}{2} \int d^2\mathbf{r} \ K^* |\nabla\phi|^2 \quad (21)$$

with the renormalized stiffness constant  $K^*$  provided the surface is in the rough phase. When the Hamiltonian is given by Eq. (21), the slope dependent part of the free energy is easily isolated to be  $K^*|\mathbf{m}|^2/(2\beta)$  from a transformation  $\phi(\mathbf{r}) \rightarrow \phi(\mathbf{r}) - \mathbf{m} \cdot \mathbf{r}$  so that the Hessian of  $\sigma(\mathbf{m})$  is simply given by  $(K^*/\beta)^2$ . Thus from the scale-invariant property in Eq. (20), the Hessian of the original system is also given by

$$\text{H}[\sigma(\mathbf{m})] = \left( \frac{K^*}{\beta} \right)^2 . \quad (22)$$

In general, the stiffness constant in Eq. (13) may be a tensor  $K_{\alpha,\beta}$  ( $\alpha, \beta = 1, 2$ ). Following the same analysis, one can easily find that  $\mathcal{P}'$  and  $G$  in Eq. (19) do not couple to  $\mathbf{m}$  either and Eq. (21) is replaced by

$$\beta\mathcal{H}^* = \frac{1}{2} \int d^2\mathbf{r} \sum_{\alpha,\beta} K_{\alpha,\beta}^* \left( \frac{\partial\phi}{\partial x_\alpha} \right) \left( \frac{\partial\phi}{\partial x_\beta} \right), \quad (23)$$

where  $K_{\alpha,\beta}^*$  is the fixed-point value of  $K_{\alpha,\beta}$ . The Hessian of the free energy is also obtained from the scale-invariant property, which yields that

$$\mathrm{H}[\sigma(\mathbf{m})] = \frac{\det(K_{\alpha,\beta}^*)}{\beta^2}. \quad (24)$$

The stiffness constant is not a good quantity since it depends on the scale of the field  $\phi$ . So it is convenient to use the Gaussian coupling constant  $g$  which is defined as the coupling constant of the Gaussian model with the Hamiltonian

$$\beta\mathcal{H}_G = \frac{g}{4\pi} \int d^2\mathbf{r} |\nabla\varphi|^2, \quad (25)$$

where the periodicity of the field  $\varphi$  is set to  $2\pi$  [19]. The periodicity of the field  $\phi$  is  $a_3$ . So it is converted to  $2\pi$  by rescaling  $\varphi = 2\pi\phi/a_3$ . After a rotation and rescale of coordinates, the Hamiltonian (23) is transformed to the form of Eq. (25) with the Gaussian coupling constant given by

$$g = 2\pi \sqrt{\det(K_{\alpha,\beta}^*)} \left( \frac{a_3}{2\pi} \right)^2. \quad (26)$$

Using Eq. (26) in Eq. (24) and  $\mathrm{H}[f(\mathbf{h})] = 1/\mathrm{H}[\sigma(\mathbf{m})]$ , one obtains that the Hessian of the free energy is given by the Gaussian coupling constant as

$$\mathrm{H}[f(\mathbf{h})] = \left[ \left( \frac{a_3^2}{k_B T} \right) \frac{1}{2\pi g} \right]^2. \quad (27)$$

The exact result of the six-vertex model in Eq. (6) is recovered since  $a_3 = 2d$  in that case.

Combining Eqs. (3) and (27), one finally obtains the universal relation between the surface curvature of the ECS and the Gaussian coupling constant in the entire rough phase

$$\kappa = \frac{2}{\pi} \frac{\lambda d^2}{k_B T} \left( \frac{p^2}{4g} \right), \quad (28)$$

where  $a_3 = pd$  is used. Equations (27) and (28) are the main results of this paper. For fcc (110) surfaces there are two equivalent crystal planes ( $p = 2$ ). Inserting  $p = 2$  in Eqs. (27) and (28), one reproduces the exact results of Eqs. (6) and (8).

### III. NUMERICAL STUDIES OF THE RSOS MODEL

In the previous section, we presented RG arguments for the relation between the Gaussian coupling constant and the Hessian of the free energy. It is obtained from the observation that the Hessian of the free energy is a scale-invariant quantity. In this section we test the validity of Eq. (27) in the RSOS model on a square lattice (denoted by  $\mathcal{L}$ ) by comparing the Gaussian coupling constant obtained from the FSS amplitudes of the transfer matrix spectra and the value obtained from the Hessian of the free energy, using Eq. (27).

The RSOS model describes the surface of sc crystals viewed from the [001] direction. The Hamiltonian for the RSOS model with the surface-tilting field  $\mathbf{h} = (h_1, h_2)$  is given by

$$\mathcal{H}_{\text{RSOS}} = K \sum_{\langle i, j \rangle} \delta(|z_i - z_j| - 1) - h_1 \sum_i (z_{i+\mathbf{e}_1} - z_i) - h_2 \sum_i (z_{i+\mathbf{e}_2} - z_i), \quad (29)$$

where  $z_i$  is the integer-valued height variable at site  $i$  in  $\mathcal{L}$ ,  $K$  is the step energy,  $\langle i, j \rangle$  denotes the pair of nearest-neighbor sites, and  $\mathbf{e}_1(\mathbf{e}_2)$  is the unit vector in 1 (2) direction. The height differences between nearest-neighbor sites are restricted to 0 and  $\pm 1$ . (In this section, length and energy are measured in units of lattice constant and  $k_B T$ , respectively. So all quantities are dimensionless.) The RSOS model with  $\mathbf{h} = 0$  displays a roughening transition at  $K = K_c \sim 0.633$  and  $g = 1/4$  at the roughening transition [20]. There is one equivalent crystal plane parallel to the (001) surface. This means that the RSOS model represents a  $p = 1$  case among the general cases discussed in Sec. II.

Height configurations of the RSOS model can be mapped to arrow configurations on bonds of the dual lattice denoted by  $\mathcal{L}_D$ . If there is no step across a bond in  $\mathcal{L}_D$ , no arrow is assigned to the bond. And if there is a step, an arrow is assigned in such a way that the height at the right-hand side of the arrow is higher than the other side by 1. Since there are no dislocations, the number of inward and outward arrows at each vertex should be equal (the so-called ice rule). There are nineteen vertex configurations satisfying the ice rule. So the RSOS model is equivalent to the 19-vertex model. The vertical (horizontal) slope corresponds to a net imbalance between left-right (up-down) arrows.

A row-to-row transfer matrix  $\mathbf{T}$  is easily constructed. The partition function on a lattice of size  $N \times M$  can be written as  $Z = \text{Tr } \mathbf{T}^M$ . If one uses the PBC for the arrow variables in the  $N$  direction, the net number  $Q$  of up arrows in each row of vertical bonds is the same in all rows due to the ice rule. So the transfer matrix is separated into blocks of the form

$$\mathbf{T} = \bigoplus_Q e^{h_1 Q} \mathbf{T}_Q,$$

where  $\mathbf{T}_Q$  operates on the  $Q$ th sector, defined by the set of arrow configurations with net number  $Q$  of up arrows ( $Q = -N, -N + 1, \dots, N$ ). The largest eigenvalue of  $\mathbf{T}_Q$  will be denoted by  $\Lambda_Q = \exp[-E_Q(N)]$  and  $E_Q(N)$  will be called the ground-state energy in the sector  $Q$ . In the limit  $N, M \rightarrow \infty$ , the free energy  $e(m_1, h_2)$  as a function of the horizontal slope  $m_1 = Q/N$  and the vertical surface-tilting field  $h_2$  is given by

$$e(m_1, h_2) = \lim_{N \rightarrow \infty} \frac{E_{m_1 N}(N)}{N}.$$

It is related to the free energy  $f(\mathbf{h})$  through the Legendre transform

$$f(\mathbf{h}) = \min_{-1 \leq m_1 \leq 1} \{e(m_1, h_2) - h_1 m_1\}$$

and equilibrium values of  $m_1$  and  $h_1$  are related by  $h_1 = \partial e(m_1, h_2) / \partial m_1$ .

It is well known that for a rough surface with average horizontal slope  $m_1$  the transfer matrix spectra follow the FSS form

$$E_Q(N) = N e(m_1, h_2) - \frac{\pi \zeta'' c}{6N}, \quad (30)$$

$$E_{Q \pm n}(N) = E_Q \pm n h_1(m_1, h_2) + \frac{2\pi \zeta''}{N} \frac{n^2 g}{2}, \quad (31)$$

where  $Q = m_1 N$ ,  $c = 1$  is the central charge for the rough phase,  $\zeta''$  is the imaginary part of the anisotropy factor, and  $g$  is the Gaussian coupling constant [9]. To obtain an estimate for  $g$ , one has to know the value of  $\zeta''$ . It can be obtained from Eq. (30) using the two ground state energies  $E_Q(N)$  and  $E_{Q'}(N')$  for two values of strip width  $N$  and  $N'$  chosen to satisfy the conditions  $Q = m_1 N$  and  $Q' = m_1 N'$ . Combining Eqs. (30) and (31), one can obtain the following estimate  $g_{\text{FSS}}(N)$  for  $g$

$$g_{\text{FSS}}(N) = \frac{N(N^2 - N'^2)}{12NN'} \left( \frac{E_{Q+1}(N) + E_{Q-1}(N) - 2E_Q(N)}{N'E_Q(N) - NE_{Q'}(N')} \right). \quad (32)$$

On the other hand if the relation (27) holds, it can be obtained from the relation

$$g_{\text{H}}(N) = \frac{1}{2\pi\sqrt{\text{H}[f(\mathbf{h})]}} \quad (33)$$

as well, where  $\text{H}$  is the Hessian of the free energy in dimensionless form. The Hessian of  $f$  is directly obtained from the partial derivatives of  $e$ :

$$\text{H}[f(\mathbf{h})] = -\frac{e_{h_2, h_2}}{e_{m_1, m_1}}.$$

The partial derivatives are evaluated numerically as

$$\begin{aligned} \frac{\partial^2 e}{\partial m_1^2} &= N(E_{Q+1} + E_{Q-1} - 2E_Q), \\ \frac{\partial^2 e}{\partial h_2^2} &= \frac{(E_Q(h_2 + \delta h_2) + E_Q(h_2 - \delta h_2) - 2E_Q(h_2))}{N(\delta h_2)^2}, \end{aligned}$$

where we choose  $\delta h_2 = 0.001$ . This procedure gives estimates  $g_{\text{H}}(N)$  for  $g$ . We use the subscripts in  $g$  to show how they are obtained.

Estimates for  $g$  obtained in these two ways are shown in Fig. 2, where a data point represents a pair of values  $(g_{\text{H}}(N), g_{\text{FSS}}(N))$ . Figure 2 (a) shows the results for  $m_1 = h_2 = 0.0$ , and  $K = 0.2, 0.4$ , and  $0.6$ . For  $m_1 = 0$ ,  $g_{\text{FSS}}(N)$  is obtained from Eq. (32) by choosing  $Q = Q' = 0$  and  $N' = N - 1$ . For each  $K$ , data shown are for the strip widths  $N = 4, 5, \dots, 10$  from left to right. A similar plot is shown in Fig. 2 (b) for  $m_1 = 1/2$ ,  $K = 0.4$ , and  $h_2 = 0.1, 0.15, 0.2, 0.25$ , and  $0.3$ . For these cases,  $N'$  in Eq. (32) is chosen to be  $N - 2$  and the strip widths  $N$  are  $6, 8$ , and  $10$  from left to right. In all cases, they converge to the same values, i.e., the data points approach the line  $g_{\text{H}} = g_{\text{FSS}}$  denoted by a broken line as  $N$  increases. The inset in Fig. 2 (a) shows the estimates for  $m_1 = h_2 = 0.0$ , and  $K = \ln[(\sqrt{5} + 1)/2]$ , where the exact value of  $g$  is known to be  $1/5$  from the self-dual property of the RSOS model [20]. Both quantities converge excellently to the exact value. The fact that  $g_{\text{H}}$  and  $g_{\text{FSS}}$  converge to the same value implies that the relation (27) holds in the RSOS model. Furthermore, as can be seen in Fig. 2,  $g_{\text{H}}$  shows better convergence

than  $g_{\text{FSS}}$ . In addition to the better convergence property,  $g_{\text{H}}$  provides a more convenient way of estimating  $g$  than the standard FSS study of the transfer matrix spectra. To obtain the estimate for  $\zeta''$  one should have two ground-state energies at different strip widths with the same value of  $m_1 = Q/N$ . But it is difficult to find a set of integer values of  $N$  and  $Q$  which gives the same value of  $m_1$ . On the other hand, to obtain  $g_{\text{H}}$ , one needs to evaluate the largest eigenvalues for a single value of  $N$ . So the relation (27) presents an efficient and convenient method to study the scaling behavior of the rough phase.

#### IV. DISCUSSIONS AND SUMMARY

In this paper, we introduce general models for crystal surfaces and derive, using the RG arguments, the relation (27) between the Gaussian coupling constant which determines the strength of critical fluctuations of the rough surface and the Hessian of the free energy. Combined with the theory of the ECS, it relates the surface curvature of the rounded region to the Gaussian coupling constant. In particular when applied to the phase transition point, it explains the universal curvature jump  $(\Delta\kappa)_{\text{KT}}$  at the roughening transition. The roughening transition takes place when the SG term in Eq. (13) becomes relevant. The RG calculations for that Hamiltonian shows that it has a scaling dimension  $x_p = p^2/(2g)$  [16], which becomes 2 at the roughening transition, i.e.,  $g = g_{\text{KT}} \equiv p^2/4$ . So one obtains the universal curvature jump

$$(\Delta\kappa)_{\text{KT}} = \frac{2}{\pi} \frac{\lambda d^2}{k_B T_R} \frac{p^2}{4g_{\text{KT}}} = \frac{2}{\pi} \frac{\lambda d^2}{k_B T_R}. \quad (34)$$

As examples, the RSOS model ( $p = 1$ ), the BCSOS model ( $p = 2$ ), and the triangular-Ising solid-on-solid (TISOS) model ( $p = 3$ ) [21] have the Gaussian coupling constants  $g = 1/4, 1$ , and,  $9/4$ , respectively, at the roughening transition points [20,9,15] and hence in each the universal curvature jump by the same amount.

Below the roughening transition, there appears a facet which is separated from the rounded regions by the PT transition line. Near the PT transition systems become extremely

anisotropic [22] and no conventional RG theory has been developed for the value of  $g$  at the transition points. Instead, the surface near the PT transition is studied using a random walk or free-fermion model [13], which predicts the universal curvature jump  $(\Delta\kappa)_{\text{PT}}$  in Eq. (5). Combining it with Eq. (28), one can see that the Gaussian coupling constant should be  $g_{\text{PT}} = 2g_{\text{KT}}$  at the PT transition points. Using that property, the PT transition point can be located accurately. In the RSOS model case, it is expected that  $g = 1/2$  at the sc (001) facet boundary. In Fig. 3 we present  $g_{\text{FSS}}(N)$  and  $g_{\text{H}}(N)$  for a surface whose horizontal slope is fixed to 0 ( $m_1 = 0$ ) for several values of  $h_2$  below the roughening temperature. The surface remains flat below a critical value of the surface-tilting field  $h_c$ . Above  $h_c$  the surface becomes tilted rough. The critical value of  $h_2$  can be accurately determined from the condition that  $g = 1/2$  at the transition. The insets of Figs. 3(a) and (b) show the estimates  $h_c(N)$  for  $h_c$  obtained from the condition  $g_{\text{FSS}}(N) = 1/2$  and  $g_{\text{H}}(N) = 1/2$ , respectively. Like the Gaussian coupling constant,  $h_c(N)$  obtained from  $g_{\text{H}}$  have less FSS corrections than those from  $g_{\text{FSS}}$ . The critical value  $h_c$  at  $K = 1.0$  is estimated as  $0.30 \pm 0.01$  (marked by arrows in the insets of Fig. 3) using polynomial fitting in  $\frac{1}{N}$ , which is consistent with a value obtained from an alternative way [23].

In summary, we derived the universal relation between the Hessian of the free energy and the Gaussian coupling constant in the rough phase of general surface model using RG arguments. It relates the surface curvature at the rounded region of the ECS to the universal quantity. Especially if it is applied to the phase transition points, it gives a clear understanding of the universal curvature jumps. The validity of the relation is checked in the RSOS model numerically. From the numerical results, it was found that the values of the Hessian have less finite-size corrections than the scaling dimensions obtained from the standard FSS theory. So, in practical points of view, this fact provides a better way in studying the scaling behaviors of the rough phase and the phase transitions in crystal surfaces.

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- [23] The facet boundary is also obtained from the first derivatives of the free energy,  $h_{\pm} = \partial e / \partial m_1|_{m_1=0^{\pm}}$ , which give the upper and lower parts of the facet boundary as a function of  $h_2$ . At the critical value of  $h_2$ ,  $h_+$  and  $h_-$  merge into a single value, i.e.,  $h_+(h_c) = h_-(h_c) = 0$ . Since the RSOS model is symmetric under the change of  $h_1 \leftrightarrow h_2$ ,  $h_c$ , the critical value of  $h_2$  at  $h_1 = 0$ , is equal to the critical value of  $h_1$  at  $h_2 = 0$ . So  $h_c$  can be obtained from extrapolation of finite size data for  $h_+(h_2 = 0)$ .

## Figure Captions

**Figure 1** Shown are the sc crystal on a substrate parallel to the (001) plane (a), the bcc crystal on a substrate parallel to the (001) plane (b), and the sc crystal on a substrate parallel to the (111) plane (c). The projected lattice points on to the substrates form 2-dimensional lattices and their sublattice structure is shown.

**Figure 2** The Gaussian coupling constants obtained from two different methods at  $m_1 = h_2 = 0$ , and  $K = 0.2, 0.4$ , and  $0.6$  (a) and at  $m_1 = 1/2$ ,  $K = 0.4$ , and  $h_2 = 0.1, 0.15, 0.2, 0.25$ , and  $0.3$  (b) are compared. The data are obtained from numerical diagonalizations of the transfer matrix for strip width  $N = 4, 5, \dots, 10$  in (a) and  $N = 6, 8$  and  $10$  in (b). The inset in (a) shows  $g_H$  and  $g_{FSS}$  at  $m_1 = h_2 = 0$ , and  $K = \ln[(\sqrt{5} + 1)/2]$  where the exact value of  $g$  is known to be  $1/5$ , whose location is indicated by the arrow. They show the converging behaviors to the exact value. The lines are guides to eyes.

**Figure 3** The Gaussian coupling constants  $g_{FSS}$  (a) and  $g_H$  (b) are shown at  $m_1 = 0.0$  and  $K = 1.0 > K_c$  for several values of  $h_2$ . The insets show the estimates for the critical values of  $h_2$  which are obtained by solving  $g = 1/2$  numerically. The extrapolated values for  $h_c$  are marked by arrows. The lines are guides to eyes.

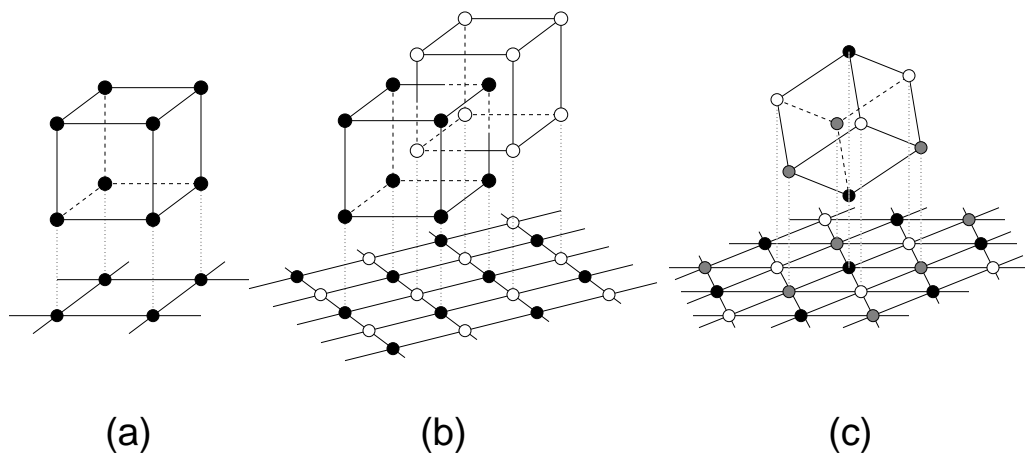


Figure 1 of Noh and Kim

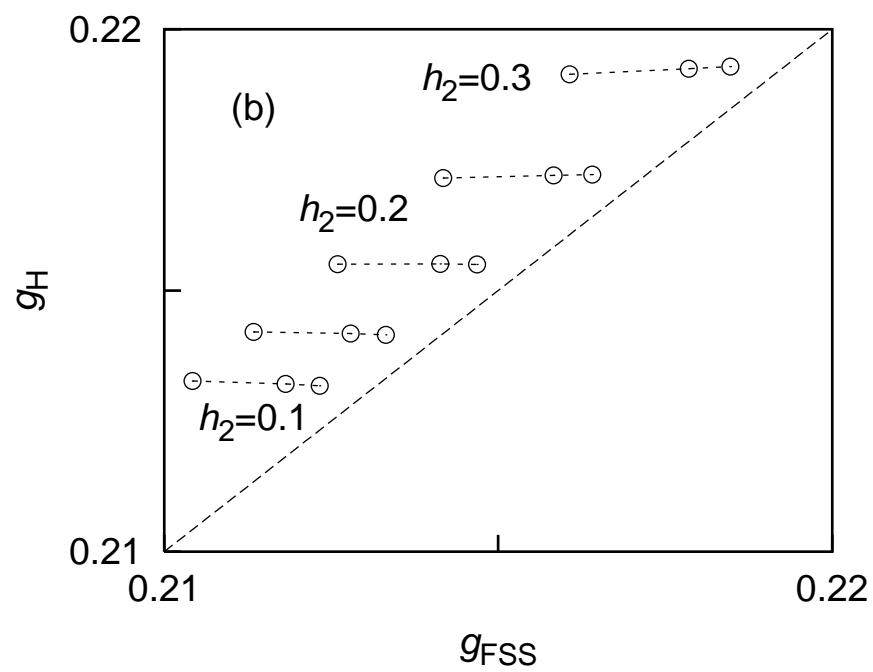
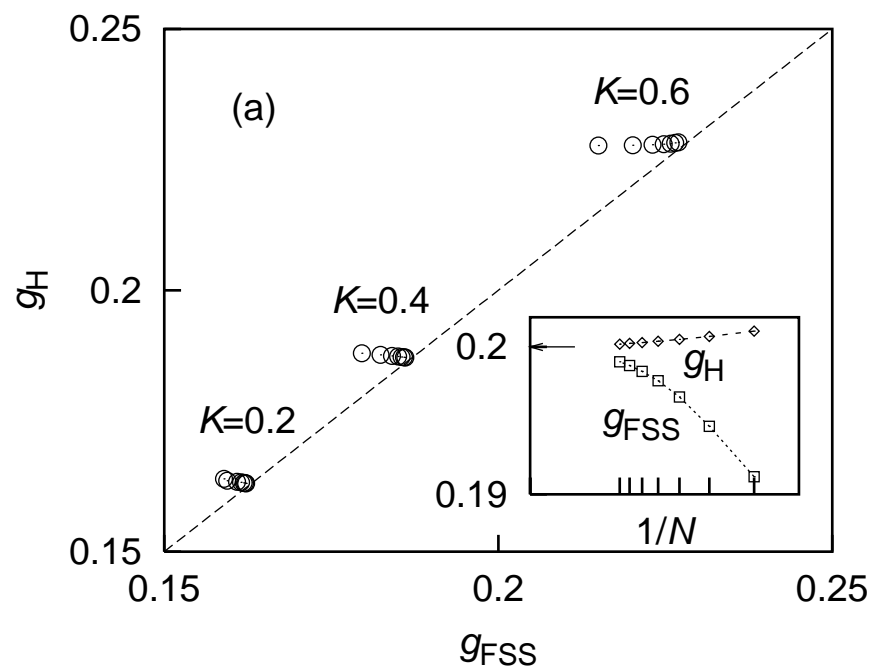


Figure 2 of Noh and Kim

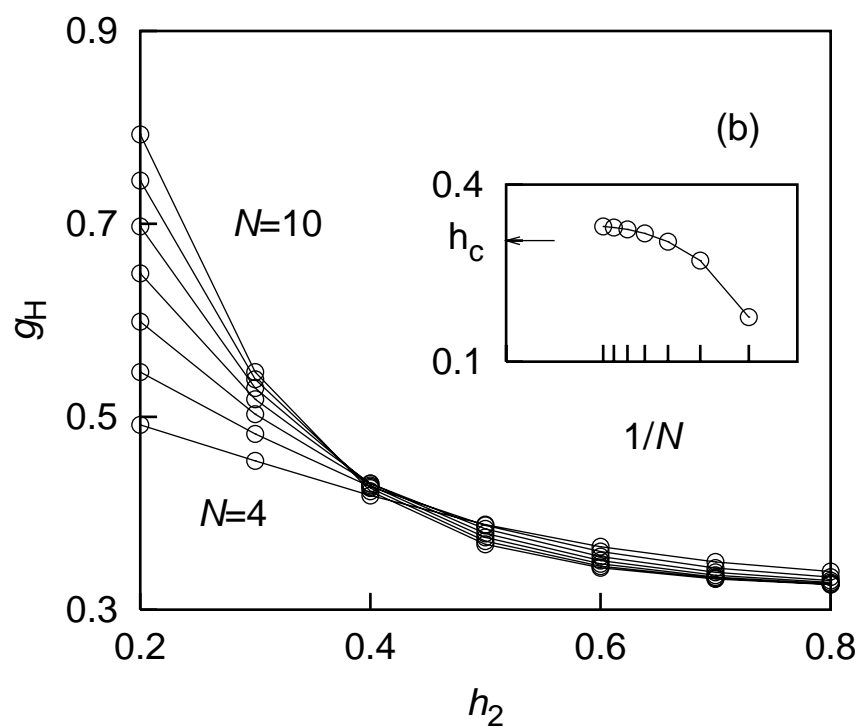
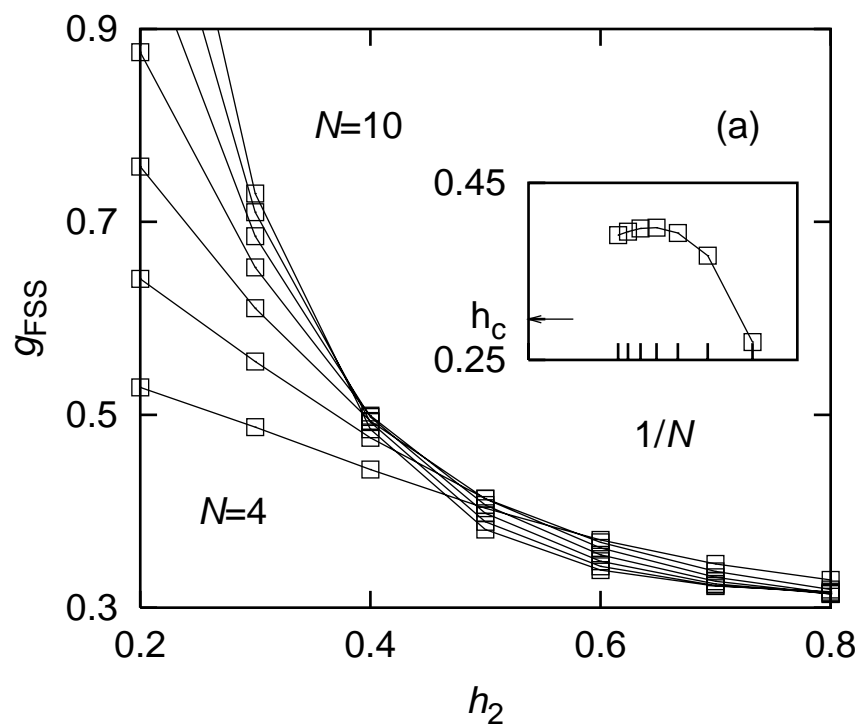


Figure 3 of Noh and Kim